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Molecular beam epitaxial growth and characterization of coherent α-Al_2O_3/Ga_2O_3 superlattices on r-plane sapphire

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Abstract

In order to explore and encourage the study on α-$(Al_xGa_{1-x})_2O_3$-alloy-based heterostructures, coherent α-Al_2O_3/Ga_2O_3 superlattices without misfit dislocations were fabricated and characterized for the first time. We found that crystallinity of the superlattices was strongly depend on the thickness of α-Ga_2O_3 layer, whose critical thickness was as small as ~1 nm. We also revealed the band-alignment of the α-Al_2O_3/Ga_2O_3 with conduction- and valence-band offsets of 2.7 and 0.3 eV, respectively.

1. Introduction

Recently, corundum structured α-Ga_2O_3 has attracted attention as an ultra-wide-band-gap semiconductor for the future application of high-power and deep-UV devices. Among the studies, research and development on α-$(Al_xGa_{1-x})_2O_3$-based heterostructures have also gathered interest owing to a wide band-gap tuning range from 5.3 to 8.8 eV. In particular, strong quantum effects are expected in α-Al_2O_3/Ga_2O_3 heterostructures because of the large difference in their band-gaps (E_g). However, fabrication of the heterostructures having coherent interfaces is challenging due to the large lattice mismatches (4.8 and 3.4% along the a- and c-axes, respectively).

In this study, we therefore fabricated α-Al_2O_3/Ga_2O_3 superlattices (SLs) by molecular beam epitaxy (MBE) and characterized them with various methods [1].

2. Growth of coherent α-Al_2O_3/Ga_2O_3 superlattices

Ten-period α-Al_2O_3/Ga_2O_3 SLs were grown on isostructural r-plane sapphire by oxygen-radical-assisted MBE. To evaluate the α-Ga_2O_3 layer thickness (d_{Ga}) dependence of crystallinity, three samples (A, B, and C) with different d_{Ga} were fabricated. The each layer thickness of the samples measured with X-ray refractivity (XRR) are listed in Table I.

Table I. d_{Ga} and α-Al_2O_3 layer thickness (d_{Al}) of the SLs.

	A	B	C
d_{Ga} (nm)	0.5	1.0	1.3
d_{Al} (nm)	5.8	6.1	6.0

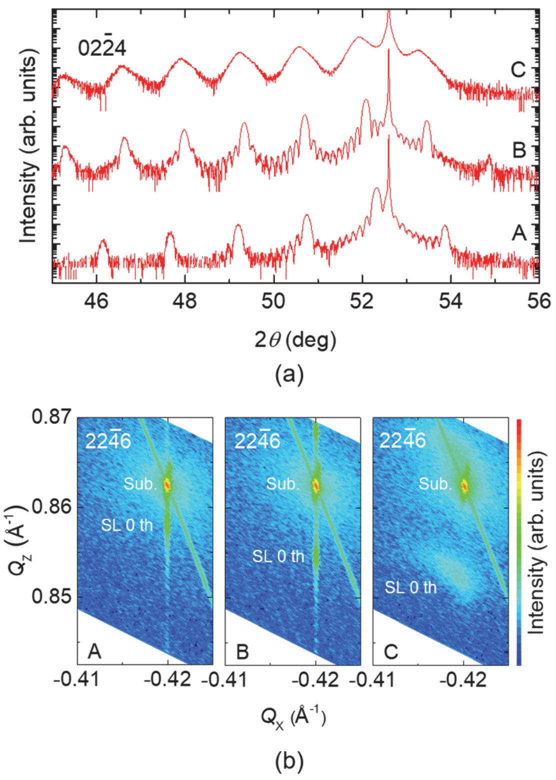

Fig. 1 (a) out-of-plane XRD patterns and (b) asymmetric XRD reciprocal space maps (RSMs) of the samples.

Figures 1(a) and (b) show summery of X-ray diffraction (XRD) characterization for the SLs. For the sample A and B, we can see satellite peaks with fringes in the θ-2θ patterns [Fig. 1(a)] and asymmetric SL peaks with the same in-plane reciprocal lattice length as the substrate in the RSMs [Fig. 1(b)], indicating highly crystalline coherent SLs. In contrast, corresponding XRD data of sample C indicate the partially related poor crystalline SL. These results suggest that α-Al_2O_3/Ga_2O_3 SLs maintained structural coherence with the sapphire substrate up to d_{Ga} ~ 1 nm (samples A and B) but relaxed when d_{Ga} surpassed ~ 1 nm (sample C) owing to the large compressive strain in the α-Ga_2O_3 layer. The critical thickness of ~ 1 nm coincides with the reported value for single α-Ga_2O_3 films on sapphire substrates [2].

3. Cross-sectional observation of the coherent SL

To observe the crystal lattices of the SL, cross-sectional scanning transmission electron microscopy (STEM) was carried out for the sample B. Figure 2(a) shows high-angle annular dark-field (HAADF) STEM image, where we can see metal atom arrays corresponding to the corundum structure [See Fig. 2(b)]. When we closely look the figure, we also notice that the plane array of Ga (brighter) perfectly matched with that of Al (darker) at the interfaces, which suggests that the coherent interfaces have no misfit dislocations.

4. Evaluation of band-alignment at the heterointerface

Having succeeded the fabrication of the coherent α-Ga_2O_3/Al_2O_3 SLs, we then evaluated the band alignment at the heterointerface using X-ray photoemission spectroscopy (XPS). For this purpose, we additionally grew an α-Al_2O_3 homoepitaxial film (8.8 nm) and a five-period α-Ga_2O_3 (0.9 nm)/Al_2O_3 (26.3 nm) coherent SL on r-plane sapphire substrates and confirmed their structural coherency again through XRD measurement. Note that the top layer of the SL is constructed with α-Ga_2O_3.

Valence-band offset ($\varDelta E_V$) was first extracted by analyzing XPS spectra near core levels and valence band maximums (VBMs) as shown in Fig. 3(a). Assuming that the valance-band edge of the SL is equal to that of the coherent α-Ga_2O_3 layer, $\varDelta E_V$ can be obtained through the comparison of the differences in energy labeled in the figure as follows:

$$\varDelta E_V = (102.6–71.0–31.3) \text{ eV} = 0.3 \text{ eV}.$$

Next, E_g of the coherently grown α-Al_2O_3 and α-Ga_2O_3 layers were obtained from the XPS O 1*s* loss structures, as shown in Fig. 3(b). The measured E_g of α-Ga_2O_3 and α-Al_2O_3 were 5.7 and 8.7 eV, respectively. Finally, conduction-band offset can be calculated using $\varDelta E_V$ and E_g as follows:

$$\varDelta E_C = (8.7–5.7–0.3) \text{ eV} = 2.7 \text{ eV}.$$

The $\varDelta E_C$ was larger compared to $\varDelta E_V$, and similar trend is also reported for α-Ga_2O_3/$(Al_xGa_{1-x})_2O_3$ interface ($0.1 \le x \le 0.8$) [3]. This trend is explained by the common feature of metal oxides that the top of the valence bands are mainly consisted with O 2*p* orbitals and are less sensitive to changes in cations.

5. Conclusions

We successfully fabricate coherent α-Al_2O_3/Ga_2O_3 SLs on r-plane sapphire by MBE, and confirmed their layered and epitaxial structures using XRR, XRD, and STEM techniques. We also revealed the band-alignment at the coherent heterojunction interface with XPS. Our provided results will contribute for further development of α-$(Al_xGa_{1-x})_2O$-based heterostructure studies.

Acknowledgements

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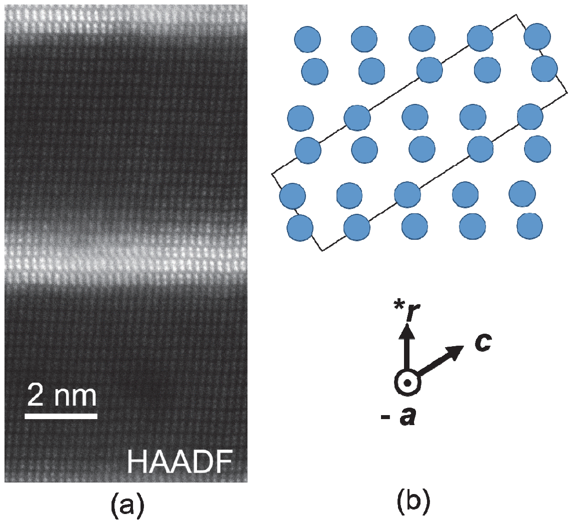

Fig. 2 (a) HAADF-STEM image of the SL sample B. (b) Metal atom positions (circles) of the corundum structure around the unit cell (solid line).

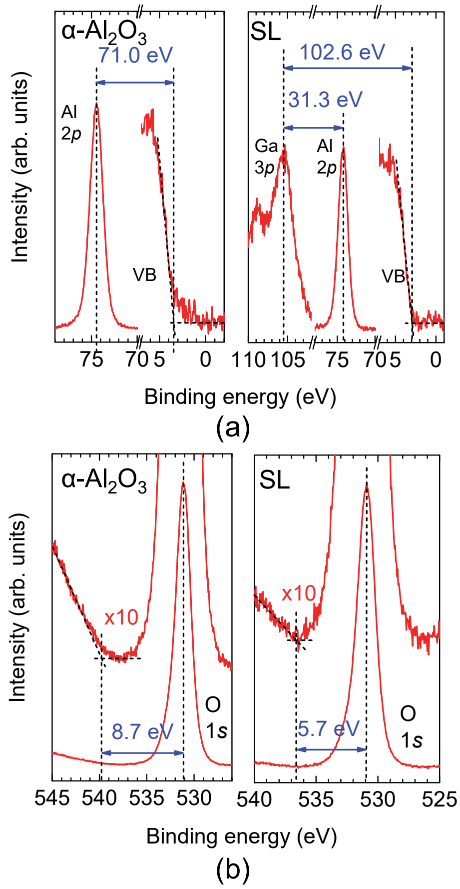

Fig. 3 XPS spectra near (a) core levels (Al 2*p* and Ga $3p_{3/2}$) and VBMs and (b) O 1*s* for the α-Al_2O_3 homoepitaxial film and the SL.

References

[1] T. Oshima et al., Appl. Phys. Express in press (2018).
[2] Z. Cheng et al., Appl. Phys. Lett. **111**, 162104 (2017).
[3] T. Uchida et al., Jpn. J. Appl. Phys. **57**, 40314 (2018).